

**Supplementary data 2.** Elementary reactions involved in the microkinetic modelling. \* and \_g denote surface and gas-phase species, respectively.

#	Reaction	Expression
1	1.0-1.1	*_s + CH4_g <-> H-CH3* -> H* + CH3_g
2	1.0-1.2	*_s + H2_g <-> H-H* -> H2*
3	1.0-2.3a	*_s + CH3_g -> CH3*
4	1.0-2.4a	*_s + CH4_g <-> C-H4* -> HCH3*
5	1.0-2.4b	*_s + CH4_g <-> CH-H3* -> CH3H*
6	1.0-3.2	*_s + C2H2_g -> CHCH*
7	1.0-3.4c	*_s + C2H4_g -> H2CCH2*
8	1.1-1.2	H* + CH4_g <-> H2-CH3* -> H2* + CH3_g
9	1.1-3.3b	H* + C2H2_g -> CHCHH*
10	1.1-2.4a	H* + CH3_g -> HCH3*
11	1.1-2.4b	H* + CH3_g -> CH3H*
12	1.1-2.5a	H* + CH4_g <-> H-CH4* -> CH3H2*
13	1.1-3.5i	H* + C2H4_g -> H2CCH2H*
14	1.2-1.3a	H2* + CH4_g <-> H2H-CH3* -> H2H* + CH3_g
15	1.2-1.3b	H2* + CH4_g <-> HH2-CH3* -> HH2* + CH3_g
16	1.2-2.5a	H2* + CH3_g -> CH3H2*
17	1.2-2.5b	H2* + CH3_g -> CH2H3*
18	1.2-2.6	H2* + CH4_g <-> H2-CH4* -> CH3H3*
19	1.2-3.4a	H2* + C2H2_g -> C2H2H2*
20	1.2-3.4b	H2* + C2H2_g -> H2C2H2*
21	1.2-3.6a	H2* + C2H4_g -> H2C2H4*
22	1.2-3.6b	H2* + C2H4_g -> C2H4H2*
23	1.3a-3.5c	H2H* + C2H2_g -> C2H2H3*
24	1.3a-3.7a	H2H* + C2H4_g -> C2H4H3*
25	1.3b-3.5d	HH2* + C2H2_g -> CH3HCH*
26	1.3b-3.7b	HH2* + C2H4_g -> CH3H2CH2*
27	2.0-2.1	C* + CH4_g <-> CH-CH3* -> CH* + CH3_g
28	2.0-2.2c	C* + H2_g <-> H-CH* -> H2C*
29	2.0-2.2d	C* + H2_g <-> CH-H* -> CHH*
30	2.1-2.2c	CH* + CH4_g <-> CH2-CH3* -> H2C* + CH3_g
31	2.1-2.2d	CH* + CH4_g <-> CH3-CH2* -> CHH* + CH3_g
32	2.1-2.3e	CH* + H2_g <-> CH-H2* -> CHH2*
33	2.1-2.3f	CH* + H2_g <-> CH-H-H* -> CHHH*
34	2.2a-2.2b	CH2* <-> C-H-H* -> HCH*
35	2.2a-2.3a	CH2* + CH4_g <-> CH3-CH3* -> CH3* + CH3_g
36	2.2a-2.3b	CH2* + CH4_g <-> CH3-HCH2* -> HCH2* + CH3_g
37	2.2a-3.5a	CH2* + CH3_g -> CH3CH2*
38	2.2a-3.5g	CH2* + CH3_g -> CHHCH3*
39	2.2b-2.2c	HCH* <-> H-C-H* -> H2C*

40	2.2b-2.3c	$\text{HCH}^* + \text{CH}_4\text{\_g} \leftrightarrow \text{CH}_2\text{H}-\text{CH}_3^* \rightarrow \text{CH}_2\text{H}^* + \text{CH}_3\text{\_g}$
41	2.2b-2.3d	$\text{HCH}^* + \text{CH}_4\text{\_g} \leftrightarrow \text{CH}_3-\text{H}_2\text{CH}^* \rightarrow \text{H}_2\text{CH}^* + \text{CH}_3\text{\_g}$
42	2.2b-3.5c	$\text{HCH}^* + \text{CH}_3\text{\_g} \rightarrow \text{C}_2\text{H}_2\text{H}_3^*$
43	2.2b-3.5d	$\text{HCH}^* + \text{CH}_3\text{\_g} \rightarrow \text{CH}_3\text{HCH}^*$
44	2.2c-2.2d	$\text{H}_2\text{C}^* \leftrightarrow \text{HC}-\text{H}^* \rightarrow \text{CHH}^*$
45	2.2c-2.3e	$\text{H}_2\text{C}^* + \text{CH}_4\text{\_g} \leftrightarrow \text{CH}_2-\text{HCH}_3^* \rightarrow \text{CHH}_2^* + \text{CH}_3\text{\_g}$
46	2.2c-2.3f	$\text{H}_2\text{C}^* + \text{CH}_4\text{\_g} \leftrightarrow \text{HCH}-\text{HCH}_3^* \rightarrow \text{CHHH}^* + \text{CH}_3\text{\_g}$
47	2.2c-3.5h	$\text{H}_2\text{C}^* + \text{CH}_3\text{\_g} \rightarrow \text{H}_2\text{CCH}_3^*$
48	2.2c-2.4b	$\text{H}_2\text{C}^* + \text{H}_2\text{\_g} \leftrightarrow \text{CH}_2-\text{H}_2^* \rightarrow \text{CH}_3\text{H}^*$
49	2.2d-2.3f	$\text{CHH}^* + \text{CH}_4\text{\_g} \leftrightarrow \text{HCH}-\text{H}_2\text{CH}_2^* \rightarrow \text{CHHH}^* + \text{CH}_3\text{\_g}$
50	2.3a-2.3b	$\text{CH}_3^* \leftrightarrow \text{CH}_2-\text{H}^* \rightarrow \text{HCH}_2^*$
51	2.3a-2.4a	$\text{CH}_3^* + \text{CH}_4\text{\_g} \leftrightarrow \text{CH}_3-\text{HCH}_3^* \rightarrow \text{HCH}_3^* + \text{CH}_3\text{\_g}$
52	2.3b-2.3c	$\text{HCH}_2^* \leftrightarrow \text{H}-\text{CH}_2^* \rightarrow \text{CH}_2\text{H}^*$
53	2.3b-2.4a	$\text{HCH}_2^* + \text{CH}_4\text{\_g} \leftrightarrow \text{HCH}_3-\text{CH}_3^* \rightarrow \text{HCH}_3^* + \text{CH}_3\text{\_g}$
54	2.3c-2.3d	$\text{CH}_2\text{H}^* \leftrightarrow \text{HC}-\text{H}-\text{H}^* \rightarrow \text{H}_2\text{CH}^*$
55	2.3c-3.6d	$\text{CH}_2\text{H}^* + \text{CH}_3\text{\_g} \rightarrow \text{C}_2\text{H}_3\text{H}_3^*$
56	2.3d-3.6c	$\text{H}_2\text{CH}^* + \text{CH}_3\text{\_g} \rightarrow \text{CH}_3\text{HCH}_2^*$
57	2.3e-2.3f	$\text{CHH}_2^* \leftrightarrow \text{HC}-\text{H}_2^* \rightarrow \text{CHHH}^*$
58	2.3e-2.4b	$\text{CHH}_2^* + \text{CH}_4\text{\_g} \leftrightarrow \text{HCH}_2-\text{CH}_4^* \rightarrow \text{CH}_3\text{H}^* + \text{CH}_3\text{\_g}$
59	2.3f-2.4b	$\text{CHHH}^* + \text{CH}_4\text{\_g} \leftrightarrow \text{CH}_3-\text{CH}_4^* \rightarrow \text{CH}_3\text{H}^* + \text{CH}_3\text{\_g}$
60	2.3f-3.6e	$\text{CHHH}^* + \text{CH}_3\text{\_g} \rightarrow \text{H}_2\text{CCH}_3\text{H}^*$
61	2.3f-2.5a	$\text{CHHH}^* + \text{H}_2\text{\_g} \leftrightarrow \text{CH}_3-\text{H}_2^* \rightarrow \text{CH}_3\text{H}_2^*$
62	2.4b-2.5a	$\text{CH}_3\text{H}^* + \text{CH}_4\text{\_g} \leftrightarrow \text{H}_2\text{CH}_3-\text{CH}_3^* \rightarrow \text{CH}_3\text{H}_2^* + \text{CH}_3\text{\_g}$
63	2.5a-2.5b	$\text{CH}_3\text{H}_2^* \leftrightarrow \text{CH}_2-\text{H}-\text{H}_2^* \rightarrow \text{CH}_2\text{H}_3^*$
64	2.5a-2.6	$\text{CH}_3\text{H}_2^* + \text{CH}_4\text{\_g} \leftrightarrow \text{CH}_3\text{H}_3-\text{CH}_3^* \rightarrow \text{CH}_3\text{H}_3^* + \text{CH}_3\text{\_g}$
65	2.5a-3.8b	$\text{CH}_3\text{H}_2^* + \text{CH}_3\text{\_g} \rightarrow \text{CH}_3\text{H}_2\text{CH}_3^*$
66	2.5b-2.6	$\text{CH}_2\text{H}_3^* + \text{CH}_4\text{\_g} \leftrightarrow \text{CH}_3-\text{CH}_3\text{H}_3^* \rightarrow \text{CH}_3\text{H}_3^* + \text{CH}_3\text{\_g}$
67	2.5b-3.8a	$\text{CH}_2\text{H}_3^* + \text{CH}_3\text{\_g} \rightarrow \text{C}_2\text{H}_5\text{H}_3^*$
68	3.2-3.3a	$\text{CHCH}^* + \text{CH}_4\text{\_g} \leftrightarrow \text{C}_2\text{H}_3-\text{CH}_3^* \rightarrow \text{CHCH}_2^* + \text{CH}_3\text{\_g}$
69	3.2-3.3b	$\text{CHCH}^* + \text{CH}_4\text{\_g} \leftrightarrow \text{HC}_2\text{H}_2-\text{CH}_3^* \rightarrow \text{CHCHH}^* + \text{CH}_3\text{\_g}$
70	3.2-3.4a	$\text{CHCH}^* + \text{H}_2\text{\_g} \leftrightarrow \text{C}_2\text{H}_2-\text{H}_2^* \rightarrow \text{C}_2\text{H}_2\text{H}_2^*$
71	3.3a-3.4c	$\text{CHCH}_2^* + \text{CH}_4\text{\_g} \leftrightarrow \text{HC}_2\text{H}_3-\text{CH}_3^* \rightarrow \text{H}_2\text{CCH}_2^* + \text{CH}_3\text{\_g}$
72	3.3a-3.4d	$\text{CHCH}_2^* + \text{CH}_4\text{\_g} \leftrightarrow \text{H}_2\text{C}_2\text{H}_2-\text{CH}_3^* \rightarrow \text{HCCH}_2\text{H}^* + \text{CH}_3\text{\_g}$
73	3.3a-3.5f	$\text{CHCH}_2^* + \text{H}_2\text{\_g} \leftrightarrow \text{C}_2\text{H}_3-\text{H}_2^* \rightarrow \text{C}_2\text{H}_3\text{H}_2^*$
74	3.3b-3.4a	$\text{CHCHH}^* + \text{CH}_4\text{\_g} \leftrightarrow \text{H}_3\text{C}_2\text{H}-\text{CH}_3^* \rightarrow \text{C}_2\text{H}_2\text{H}_2^* + \text{CH}_3\text{\_g}$
75	3.3b-3.4d	$\text{CHCHH}^* + \text{CH}_4\text{\_g} \leftrightarrow \text{C}_2\text{H}_4-\text{CH}_3^* \rightarrow \text{HCCH}_2\text{H}^* + \text{CH}_3\text{\_g}$
76	3.4a-3.5c	$\text{C}_2\text{H}_2\text{H}_2^* + \text{CH}_4\text{\_g} \leftrightarrow \text{C}_2\text{H}_2\text{H}_3-\text{CH}_3^* \rightarrow \text{C}_2\text{H}_2\text{H}_3^* + \text{CH}_3\text{\_g}$
77	3.4a-3.5f	$\text{C}_2\text{H}_2\text{H}_2^* + \text{CH}_4\text{\_g} \leftrightarrow \text{C}_2\text{H}_3\text{H}_2-\text{CH}_3^* \rightarrow \text{C}_2\text{H}_3\text{H}_2^* + \text{CH}_3\text{\_g}$
78	3.4b-3.5d	$\text{H}_2\text{C}_2\text{H}_2^* + \text{CH}_4\text{\_g} \leftrightarrow \text{C}_2\text{H}_5-\text{CH}_3^* \rightarrow \text{CH}_3\text{HCH}^* + \text{CH}_3\text{\_g}$
79	3.4b-3.5e	$\text{H}_2\text{C}_2\text{H}_2^* + \text{CH}_4\text{\_g} \leftrightarrow \text{HC}_2\text{H}_4-\text{CH}_3^* \rightarrow \text{H}_2\text{C}_2\text{H}_3^* + \text{CH}_3\text{\_g}$
80	3.4c-3.5h	$\text{H}_2\text{CCH}_2^* + \text{CH}_4\text{\_g} \leftrightarrow \text{H}_2\text{C}_2\text{H}_3-\text{CH}_3^* \rightarrow \text{H}_2\text{CCH}_3^* + \text{CH}_3\text{\_g}$
81	3.4c-3.5i	$\text{H}_2\text{CCH}_2^* + \text{CH}_4\text{\_g} \leftrightarrow \text{H}_3\text{C}_2\text{H}_2-\text{CH}_3^* \rightarrow \text{H}_2\text{CCH}_2\text{H}^* + \text{CH}_3\text{\_g}$
82	3.4d-3.5i	$\text{HCCH}_2\text{H}^* + \text{CH}_4\text{\_g} \leftrightarrow \text{H}_4\text{C}_2\text{H}-\text{CH}_3^* \rightarrow \text{H}_2\text{CCH}_2\text{H}^* + \text{CH}_3\text{\_g}$
83	3.4d-3.5h	$\text{HCCH}_2\text{H}^* + \text{CH}_4\text{\_g} \leftrightarrow \text{H}_5\text{C}_2-\text{CH}_3^* \rightarrow \text{H}_2\text{CCH}_3^* + \text{CH}_3\text{\_g}$

84	3.5a-3.6c	$\text{CH}_3\text{CH}_2^* + \text{CH}_4\_g \leftrightarrow \text{CH}_3\text{-CH}_3\text{HCH}_2^* \rightarrow \text{CH}_3\text{HCH}_2^* + \text{CH}_3\_g$
85	3.5a-3.5d	$\text{CH}_3\text{CH}_2^* \leftrightarrow \text{CH}_3\text{-H-CH}^* \rightarrow \text{CH}_3\text{HCH}^*$
86	3.5b-3.5c	$\text{CH}_2\text{CH}_3^* \leftrightarrow \text{CH-H-CH}_3^* \rightarrow \text{C}_2\text{H}_2\text{H}_3^*$
87	3.5b-3.5g	$\text{CH}_2\text{CH}_3^* \leftrightarrow \text{C-H}_2\text{CH}_3^* \rightarrow \text{CHHCH}_3^*$
88	3.5b-3.5f	$\text{CH}_2\text{CH}_3^* \leftrightarrow \text{CH}_2\text{-H-H}_2\text{C}^* \rightarrow \text{C}_2\text{H}_3\text{H}_2^*$
89	3.5b-3.6d	$\text{CH}_2\text{CH}_3^* + \text{CH}_4\_g \leftrightarrow \text{CH}_3\text{-C}_2\text{H}_3\text{H}_3^* \rightarrow \text{C}_2\text{H}_3\text{H}_3^* + \text{CH}_3\_g$
90	3.5c-3.6d	$\text{C}_2\text{H}_2\text{H}_3^* + \text{CH}_4\_g \leftrightarrow \text{C}_2\text{H}_3\text{H}_3\text{-CH}_3^* \rightarrow \text{C}_2\text{H}_3\text{H}_3^* + \text{CH}_3\_g$
91	3.5d-3.6c	$\text{CH}_3\text{HCH}^* + \text{CH}_4\_g \leftrightarrow \text{CH}_3\text{HCH}_2\text{-CH}_3^* \rightarrow \text{CH}_3\text{HCH}_2^* + \text{CH}_3\_g$
92	3.5e-3.6c	$\text{H}_2\text{C}_2\text{H}_3^* + \text{CH}_4\_g \leftrightarrow \text{C}_2\text{H}_6\text{-CH}_3^* \rightarrow \text{CH}_3\text{HCH}_2^* + \text{CH}_3\_g$
93	3.5e-3.6a	$\text{H}_2\text{C}_2\text{H}_3^* + \text{CH}_4\_g \leftrightarrow \text{CHCH}_5\text{-CH}_3^* \rightarrow \text{H}_2\text{C}_2\text{H}_4^* + \text{CH}_3\_g$
94	3.5f-3.6d	$\text{C}_2\text{H}_3\text{H}_2^* + \text{CH}_4\_g \leftrightarrow \text{CH}_2\text{CH}_4\text{-CH}_3^* \rightarrow \text{C}_2\text{H}_3\text{H}_3^* + \text{CH}_3\_g$
95	3.5f-3.6b	$\text{C}_2\text{H}_3\text{H}_2^* + \text{CH}_4\_g \leftrightarrow \text{CH}_3\text{CH}_3\text{-CH}_3^* \rightarrow \text{C}_2\text{H}_4\text{H}_2^* + \text{CH}_3\_g$
96	3.5h-3.6e	$\text{H}_2\text{CCH}_3^* + \text{CH}_4\_g \leftrightarrow \text{CH}_4\text{CH}_2\text{-CH}_3^* \rightarrow \text{H}_2\text{CCH}_3\text{H}^* + \text{CH}_3\_g$
97	3.5h-3.7c	$\text{H}_2\text{CCH}_3^* + \text{H}_2\_g \leftrightarrow \text{C}_2\text{H}_5\text{-H}_2^* \rightarrow \text{H}_2\text{CCH}_3\text{H}_2^*$
98	3.5i-3.6b	$\text{H}_2\text{CCH}_2\text{H}^* + \text{CH}_4\_g \leftrightarrow \text{CH}_5\text{CH-CH}_3^* \rightarrow \text{C}_2\text{H}_4\text{H}_2^* + \text{CH}_3\_g$
99	3.5i-3.6e	$\text{H}_2\text{CCH}_2\text{H}^* + \text{CH}_4\_g \leftrightarrow \text{CH}_6\text{C-CH}_3^* \rightarrow \text{H}_2\text{CCH}_3\text{H}^* + \text{CH}_3\_g$
100	3.6a-3.7b	$\text{H}_2\text{C}_2\text{H}_4^* + \text{CH}_4\_g \leftrightarrow \text{CH}_3\text{-CH}_3\text{H}_2\text{CH}_2^* \rightarrow \text{CH}_3\text{H}_2\text{CH}_2^* + \text{CH}_3\_g$
101	3.6b-3.7c	$\text{C}_2\text{H}_4\text{H}_2^* + \text{CH}_4\_g \leftrightarrow \text{C}_2\text{H}_7\text{-CH}_3^* \rightarrow \text{H}_2\text{CCH}_3\text{H}_2^* + \text{CH}_3\_g$
102	3.6b-3.7a	$\text{C}_2\text{H}_4\text{H}_2^* + \text{CH}_4\_g \leftrightarrow \text{C}_2\text{H}_4\text{H}_3\text{-CH}_3^* \rightarrow \text{C}_2\text{H}_4\text{H}_3^* + \text{CH}_3\_g$
103	3.6c-3.7b	$\text{CH}_3\text{HCH}_2^* + \text{CH}_4\_g \leftrightarrow \text{CH}_3\text{H}_2\text{CH}_2\text{-CH}_3^* \rightarrow \text{CH}_3\text{H}_2\text{CH}_2^* + \text{CH}_3\_g$
104	3.6d-3.7a	$\text{C}_2\text{H}_3\text{H}_3^* + \text{CH}_4\_g \leftrightarrow \text{CH}_3\text{-C}_2\text{H}_4\text{H}_3^* \rightarrow \text{C}_2\text{H}_4\text{H}_3^* + \text{CH}_3\_g$
105	3.6e-3.7c	$\text{H}_2\text{CCH}_3\text{H}^* + \text{CH}_4\_g \leftrightarrow \text{CH}_6\text{CH-CH}_3^* \rightarrow \text{H}_2\text{CCH}_3\text{H}_2^* + \text{CH}_3\_g$
106	3.7a-3.8a	$\text{C}_2\text{H}_4\text{H}_3^* + \text{CH}_4\_g \leftrightarrow \text{CH}_3\text{-C}_2\text{H}_5\text{H}_3^* \rightarrow \text{C}_2\text{H}_5\text{H}_3^* + \text{CH}_3\_g$
107	3.7b-3.8b	$\text{CH}_3\text{H}_2\text{CH}_2^* + \text{CH}_4\_g \leftrightarrow \text{CH}_3\text{H}_2\text{CH}_3\text{-CH}_3^* \rightarrow \text{CH}_3\text{H}_2\text{CH}_3^* + \text{CH}_3\_g$
108	3.7c-3.8a	$\text{H}_2\text{CCH}_3\text{H}_2^* + \text{CH}_4\_g \leftrightarrow \text{C}_2\text{H}_8\text{-CH}_3^* \rightarrow \text{C}_2\text{H}_5\text{H}_3^* + \text{CH}_3\_g$